

Exact diagonalization of the truncated Bogoliubov Hamiltonian

Loris Ferrari

Department of Physics and Astronomy of the University (DIFA)
Via Irnerio, 46, 40127, Bologna, Italy

October 25, 2016

Abstract

The present short note is simply intended to communicate that I have analytically diagonalized the Bogoliubov truncated Hamiltonian H_c [1, 2], in an interacting bosonic gas. This is the natural prosecution of my work [3], now denoted as (I), where the diagonalization was performed only in the subspace corresponding to zero momentum collective excitations (CE).

PACS: 05.30.Jp; 21.60.Fw; 67.85.Hj; 03.75.Nt

Key words: Boson systems; Interacting Boson models; Bose-Einstein condensates; Superfluidity.

e-mail: loris.ferrari@unibo.it telephone: ++39-051-2095109

The Hamiltonian under consideration is:

$$H_c = \frac{\overbrace{\hat{u}(0)N^2}^{E_{in}}}{2} + \sum_{\mathbf{k} \neq 0} \left[\overbrace{\left[\mathcal{T}(k) + \tilde{N}_{in} \hat{u}(k) \right]}^{\tilde{\epsilon}_1(k)} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \right. \\ \left. + \frac{1}{2} \sum_{\mathbf{k} \neq 0} \hat{u}(k) \left[b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger (b_0)^2 + b_{\mathbf{k}} b_{-\mathbf{k}} (b_0^\dagger)^2 \right] \right], \quad (1)$$

where $b_{\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$ create and destroy a spinless boson in the free-particle state $\langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k} \cdot \mathbf{r}} / \sqrt{V}$ and

$$\hat{u}(q) = \frac{1}{V} \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} u(r),$$

is the Fourier transform of the *repulsive* interaction energy $u(r)$ (> 0). $\mathcal{T}(k) = \hbar^2 k^2 / (2M)$ is the kinetic energy. The number operator $\tilde{N}_{in} = b_0^\dagger b_0$ refers to the bosons in the ground state, while $\tilde{N}_{out} = \sum_{\mathbf{k} \neq \mathbf{0}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ will be used to numerate bosons in the excited states. Overtilded symbols indicate operators, to avoid confusion with their (non overtilded) eigenvalues.

The base I shall use for diagonalizing H_c is formed by Fock states:

$$|j, \mathbf{k}\rangle_\eta = \frac{(b_0^\dagger)^{N-2j-\eta}}{\sqrt{(N-2j-\eta)!}} \frac{(b_{\mathbf{k}}^\dagger)^{j+\eta} (b_{-\mathbf{k}}^\dagger)^j}{\sqrt{j!(j+\eta)!}} |\emptyset\rangle, \quad (2)$$

with $j + \eta$ (real) bosons in $|\mathbf{k}\rangle$, j bosons in $|\mathbf{-k}\rangle$ and $N - 2j - \eta$ bosons in $|\mathbf{0}\rangle$, so that the total momentum is, manifestly, $\eta \hbar \mathbf{k}$.

Following the method developed in (I), I take advantage of the dependence on $k = |\mathbf{k}|$ of $\mathcal{T}(k)$ and $\hat{u}(k)$, to express the Hamiltonian H_c (eq.n (1)) as a sum of independent one-momentum Hamiltonians

$$H_c = E_{in} + \sum_{\mathbf{k} \neq \mathbf{0}} \tilde{h}_c(\mathbf{k}), \quad (3a)$$

where:

$$\begin{aligned} \tilde{h}_c(\mathbf{k}) = & \frac{1}{2} \tilde{\epsilon}_1(k) [b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}] + \\ & + \frac{1}{2} \hat{u}(k) \left[b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger (b_{\mathbf{0}})^2 + b_{\mathbf{k}} b_{-\mathbf{k}} (b_{\mathbf{0}}^\dagger)^2 \right]. \end{aligned} \quad (3b)$$

I study the *exact* eigenstates of $\tilde{h}_c(\mathbf{k})$ as linear combinations of the states eq.n (2):

$$|S, \mathbf{k}, \eta\rangle = \sum_{j=0}^{\infty} \phi_S(j, \eta) |j, \mathbf{k}\rangle_\eta, \quad (4a)$$

by solving the eigenvalue equation

$$\tilde{h}_c |S, \mathbf{k}, \eta\rangle = \mathcal{E}_S(k, \eta) |S, \mathbf{k}, \eta\rangle \quad (4b)$$

in the unknowns $\phi_S(j, \eta)$, with boundary conditions $\lim_{j \rightarrow \infty} \phi_S(j, \eta) = 0$ (necessary for normalizability) and $\phi_S(-1, \eta) = 0$ (exclusion of negative

populations)¹. It should be clear that η can be assumed non negative, without loss of generality, and represents the asymmetry in the excited states populations with opposite momentum.

I provisionally drop the dependence on \mathbf{k} , S , η , and express the energies in units of $N\hat{u}(k)$:

$$\epsilon_1 = \frac{\epsilon_1(k)}{N\hat{u}(k)}, \underline{\epsilon} = \frac{\mathcal{E}_S(k, \eta)}{N\hat{u}(k)}, \epsilon = \frac{\epsilon(k)}{N\hat{u}(k)}. \quad (5)$$

Then a slight generalization of the procedure adopted in Section 3 of (I) for equations (4a) and (3b) yields, in the TL:

$$\begin{aligned} & [\epsilon_1(2j + \eta) - 2\underline{\epsilon}] \phi(j) + \\ & + \sqrt{(j + \eta)j} \phi(j - 1) + \sqrt{(j + 1 + \eta)(j + 1)} \phi(j + 1) = 0. \end{aligned} \quad (6)$$

Thanks to the transformation:

$$\phi(j) = x^j \sqrt{\frac{(j + \eta)!}{j! \eta!}} P(j), \quad (7)$$

equation (6) yields, in turn:

$$\begin{aligned} & [\epsilon_1(2j + \eta) - 2\underline{\epsilon}] P(j) + \\ & + \frac{j}{x} P(j - 1) + x(j + 1 + \eta) P(j + 1) = 0, \end{aligned} \quad (8)$$

in the new unknowns x and $P(j)$. As shown in Section 3 of (I), a finite difference equation in the form (8) can be solved by assuming for $P(j)$ a S -degree polynomial expression:

$$P(j) = \sum_{n=0}^S C(n) j^n. \quad (9)$$

A system of $S + 2$ linear equations for the unknowns $C(j)$ then follows from the vanishing of each term proportional to j^n , with $n = 0, 1, \dots, S + 1$:

¹The reason why the sum in eq.n (4a) can be extended to ∞ , in the TL, though j cannot exceed the value $(N - \eta)/2$ is explained in detail in (I).

$$\begin{aligned}
& (\underline{\epsilon}_1 \eta - 2\underline{\mathcal{E}}) C(n) + 2\underline{\epsilon}_1 C(n-1) + \\
& + x \left[(1 + \eta) \sum_{s=n}^S C(s) \binom{n}{s} + \sum_{s=n-1}^S C(s) \binom{n}{s-1} \right] - \\
& - \frac{1}{x} \sum_{s=n-1}^S C(n) \binom{n}{s-1} (-1)^{n-s+1} = 0, \tag{10}
\end{aligned}$$

($C(S+1) = 0$ by definition). I am especially interested in the two highest order equations ($n = S+1, S$) and in the lowest order one ($n = 0$). From the system (10) one gets:

$$C(S) [2\underline{\epsilon}_1 + x + x^{-1}] = 0 \quad (n = S+1) \quad (11a)$$

$$\begin{aligned}
& C(S-1) [2\underline{\epsilon}_1 + x + x^{-1}] + \\
& + C(S) [\underline{\epsilon}_1 \eta - 2\underline{\mathcal{E}} + S(x - x^{-1}) + x(1 + \eta)] = 0 \quad (n = S) \quad (11b)
\end{aligned}$$

...

$$(\underline{\epsilon}_1 \eta - 2\underline{\mathcal{E}}) C(0) + x(1 + \eta) \sum_{s=0}^S C(s) \quad (n = 0). \quad (11c)$$

For any non vanishing value of $C(S)$, equation (11a) determines x , according to the equation $x^2 + 2x\underline{\epsilon}_1 + 1 = 0$, with the condition $|x| < 1$ (normalizability):

$$x = \underline{\epsilon} - \underline{\epsilon}_1 \quad ; \quad x^{-1} = -(\underline{\epsilon} + \underline{\epsilon}_1) \tag{12}$$

with

$$\begin{aligned}
\epsilon(k) &= \sqrt{\mathcal{T}^2(k) + 2N \widehat{u}(k) \mathcal{T}(k)} = \\
&= \frac{\hbar k}{\sqrt{2M}} \sqrt{2N \widehat{u}(k) + \frac{\hbar^2 k^2}{2M}} = \\
&= N \widehat{u}(k) \sqrt{\underline{\epsilon}_1^2 - 1} .
\end{aligned} \tag{13}$$

(remember eq.ns (5)). Then, equation (11b) determines $\underline{\mathcal{E}}$, according to the equation:

$$\underline{\epsilon}_1 \eta - 2\underline{\mathcal{E}} + S(x - x^{-1}) + x(1 + \eta) = 0 , \tag{14}$$

that, with the aid of eq.n (12) and with $k, S, \eta, N \widehat{u}(k)$ restored, yields the complete energy eigenvalues:

$$\begin{aligned}
\mathcal{E}_S(k, \eta) &= \frac{\epsilon(k)}{2} \left(\eta + \frac{1}{2} \right) + \epsilon(k) \left(S + \frac{1}{2} \right) - \\
&\quad - \underbrace{\left[\frac{\epsilon_1(k)}{2} + \frac{3\epsilon(k)}{4} \right]}_{\mathcal{E}_0(k)} \quad (S, \eta = 0, 1, \dots) ,
\end{aligned} \tag{15}$$

The algebraic structure of the eigenvalue problem (10) is fairly peculiar: equations (11a) and (11b) determine x and $\underline{\mathcal{E}}$ (i.e. the exponential decay in j and the energy eigenvalue). The still arbitrary coefficients $C(S)$ and $C(S-1)$ enter the next S equations, that can be solved for the S unknowns $C(1), C(2), \dots, C(N)$ in terms of, say, $C(0)$, that will be determined by normalization.

Finally, recalling eq.ns (9) and (7), it is easy to see that equation (11c) coincides with the boundary condition following from eq.n (6)²:

$$\phi(-1) = 0 \Rightarrow (\underline{\epsilon}_1 \eta - 2\underline{\mathcal{E}}) \phi(0) + \phi(1) \sqrt{1 + \eta} = 0 . \tag{16}$$

²The boundary condition at $j = -1$ plays an important role in selecting the eigen-solution. Actually, a different choice $\phi(j) = x^j \sqrt{j! \eta! / (j + \eta)!} P(j)$ would yield a S -degree polinomial solution for $P(j)$, just like eq.n (7), but the boundary condition $\phi(-1, \eta) = 0$ would not be satisfied.

Restoring all the relevant entries determining the state (4a), and recalling eq.ns (7), (9), one finally gets:

$$|S, \mathbf{k}, \eta\rangle = \sum_{j=0}^{\infty} x^j \sqrt{\binom{j+\eta}{j}} \overbrace{\sum_{s=0}^S C_S(s, \eta) j^s}^{\phi_S(j, \eta)} |j, \mathbf{k}\rangle_{\eta}. \quad (17)$$

The probability amplitude on the Fock states $|j, \mathbf{k}\rangle_{\eta}$ (eq.n (2)) reads, asymptotically:

$$|\phi_S(j, \eta)|^2 \rightarrow j^{2S+\eta} x^{2j}, \quad (18)$$

showing that the total number $2S+\eta$ of energy quanta $\epsilon(k)/2$ (see eq.n (15)), associated to an eigenstate eq.n (17), coincides with the highest power of j , in the limit $j \gg 1$.

Recalling that the eigenvalues (15) must be counted *twice* in the sum (3a)³, the main results of the exact diagonalization of H_c are:

- (A) The energy spectrum results from the sum of *two* independent oscillators, one with frequency $2\epsilon(k)/h$, labeled by the non negative integer S ; the other with halved frequency $\epsilon(k)/(h)$, labeled by the non negative integer η .
- (B) If, as reasonable, the quasiphonons's must behave like (massless) particles and, thereby, must carry a finite momentum, the generating oscillator is the one labeled by η and the energy of each quasiphonons is $\epsilon(k)$.

The physical consequences of these results and a comparison with the current picture of Bogoliubov/Landau CE's in the interacting boson gas will appear in a forthcoming paper.

References

- [1] N.N. Bogoliubov: *On the theory of superfluidity*, J. Phys. (USSR) **11** (1947) 23.
- [2] N.N. Bogoliubov: *About the theory of superfluidity*, Izv. Akad. Nauk USSR **11** (1947) 77.

³This point escaped from my attention in ref. [3]. A corrigendum has been sent to Physica B, to emend the error.

- [3] Loris Ferrari, *Exact Canonic Eigenstates of the truncated Bogoliubov Hamiltonian in an interacting bosons gas*, Physica B: Cond.Matt. **496**, 38-44 (2016).